CHLOROPHENOLS

CAS Registry Number: See table

Molecular Formula for chlorophenols: $C_6H_nCl_mO$ where m=1 to 5, n=1 to 4

$$X \longrightarrow X$$
 OH

x =chlorine, hydrogen, or both

Chlorophenols are typically crystalline, with solubility in ethers, alcohol, petroleum solvents, and slight to no solubility in water. Many chlorophenols have a characteristic phenolic odor. Three chlorophenols, namely 2,4,5-trichlorophenol, 2,4,6-trichlorophenol and pentachlorophenol are discussed in individual summary sheets. The monochlorophenols (m-, o-, and p-chlorophenol) and 2,3,4,6-tetrachlorophenol will be discussed in this summary sheet as representatives of this class of compounds. Only limited information could be located for each compound. Health effects information was readily available only for o-chlorophenol and 2,3,4,6-tetra-chlorophenol.

m-Chlorophenol is a crystal that is soluble in cold water (slightly), alcohol, ether, and caustic alkali solutions (Merck, 1989). It emits toxic fumes of chlorine when heated to decomposition (Sax, 1989).

o-Chlorophenol is a light amber liquid that is soluble in water (slightly), alcohol, ether, and caustic alkali solutions (Merck, 1989). It emits toxic fumes of chlorine when heated to decomposition (Sax, 1989).

p-Chlorophenol is a crystal with a characteristic phenolic odor. It is soluble in water (slightly), liquid petrolatum (slightly), alcohol, glycerin, ether, chloroform, and fixed and volatile oils (Merck, 1989). It is combustible when exposed to heat or flame and emits toxic fumes of chlorine when heated to decomposition (Sax, 1989).

2,3,4,6-Tetrachlorophenol is found as brown flakes or a sublimed mass with a strong odor. It is non-flammable, and soluble in acetone, benzene, ether, and alcohol. It emits toxic fumes of chlorine when heated to decomposition (Sax, 1987; Sax, 1989).

Physical Properties of Chlorophenols

Examples: m-chlorophenol: 3-chlorophenol

o-chlorophenol: 2-chlorophenol, 2-chloro-hydroxybenzene

p-chlorophenol: parachlorophenol, 4-chlorophenol

2,3,4,6-tetrachlorophenol: Dowicide 6, 2,4,5,6-tetrachlorophenol

	<u>m-chloro</u>	<u>o-chloro</u>	<u>p-chloro</u>	2,3,4,6-tetrachloro
CAS Registry No.:	108-43-0	95-57-8	106-48-9	58-90-2
Molecular Weight:	128.56	128.56	128.56	231.88
Boiling Point:	214.0 °C	175.0 °C	220.0 °C	164.0 °C
Melting Point:	33.5 °C	9.3 °C	4.2 - 43.7 °C	69 - 70 °C
Flash Point:	>112.0 °C	147.0 °F	20.0 °F	
Density at 45 °C:				
(water = 1)	1.245	1.2573	1.2238	1.839 (25/4 °C)
Vapor Pressure (25 °C):				
(mm Hg)	0.119	1.42	0.087	
Log Octanol/Water				
Partition Coefficient:	2.50	2.15	2.39	
Conversion Factor:	5.26	5.26	5.26	9.48
$(1 \text{ ppm} = \text{ mg/m}^3)$				
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(Sax, 1987; Sax, 1989)

SOURCES AND EMISSIONS

A. Sources

Chlorophenols are used in leather tanning and finishing. The monochlorophenols are used as synthetic intermediates for dyes and chlorinated phenols. m-Chlorophenol is reported to be formed during chlorination of sewage and p-chlorophenol is used as a denaturant for alcohol, as an antiseptic, and as a selective solvent for refining mineral. p-Chlorophenol is also formed inadvertently through chlorination of phenol-containing effluent and drinking water sources (Howard, 1990).

The primary sources that have reported emissions of chlorophenols in California are hospital services, miscellaneous wood product manufacturing, and electrical services (ARB, 1997b).

B. Emissions

The total emissions of chlorophenols from stationary sources in California are estimated to be at least 260 pounds per year, based on data reported under the Air Toxics "Hot Spots" Program (AB 2588) (ARB, 1997b).

C. Natural Occurrence

o-, m-, and p-Chlorophenol are synthetic organic compounds and have no known natural sources (Howard, 1990). Pentachlorophenol may be a product of fungus metabolism (HSDB, 1993).

AMBIENT CONCENTRATIONS

No Air Resources Board data exist for ambient measurements of chlorophenols. However, the United States Protection Agency (U.S. EPA) has compiled ambient air data from various cities for 2,4,5-trichlorophenol, 2,4,6-trichlorophenol and pentachlorophenol. For a discussion on ambient concentrations of these compounds, please see their corresponding fact sheets (U.S. EPA, 1993a).

INDOOR SOURCES AND CONCENTRATIONS

No information about the concentrations of chlorophenols was found in the readily-available literature except as discussed in the pentachlorophenol summary.

ATMOSPHERIC PERSISTENCE

For discussion on the atmospheric persistence of 2,4,5-trichlorophenol, 2,4,6-trichlorophenol and pentachlorophenol, please see their corresponding summary sheets. No information about the atmospheric half-life and lifetime of the monochlorophenols was found in the readily-available literature.

AB 2588 RISK ASSESSMENT INFORMATION

The Office of Environmental Health Hazard Assessment reviews risk assessments submitted under the Air Toxics "Hot Spots" Program. Chlorophenols contributed to the total cancer risk in 2 of the approximately 550 risk assessments reporting a total cancer risk equal to or greater than 1 in 1 million (OEHHA, 1996a).

HEALTH EFFECTS

Probable routes of human exposure to chlorophenols are inhalation, ingestion, eye and dermal contact (HSDB, 1995).

Vapors of chlorophenols are eye and respiratory tract irritants. Direct dermal contact is highly irritating. In general, exposure to the lower chlorinated phenols results in convulsions, whereas the higher chlorinated phenols are uncouplers of oxidative phosphorylation (Clayton and Clayton, 1994). Chlorophenols may be contaminated with polychloro-p-dibenzodioxins and polychlorodibenzofurans. Chlorophenols consist of many chemically distinct compounds and much

of the toxicologic information refers to the class as a whole. For example, the International Agency for Research on Cancer's (IARC) classification of possible human carcinogen (Group 2B) is based on limited human evidence for chlorophenols as a class (IARC, 1987a). The available information on 2,4,5-trichlorophenol, 2,4,6-trichlorophenol and pentachlorophenol can be found in their respective summary sheets. Information on other specific chlorophenols is given below.

o-Chlorophenol

Non-Cancer: Exposure to o-chlorophenol can lead to kidney and liver damage and intestinal hemorrhage (Clayton and Clayton, 1994). A chronic non-cancer Reference Exposure Level (REL) of 18 micrograms per cubic meter (μ g/m³) is listed for o-chlorophenol in the California Air Pollution Control Officers Association Air Toxics "Hot Spots" Program, Revised 1992 Risk Assessment Guidelines. The toxicological endpoints considered for chronic toxicity are the gastrointestinal system and liver (CAPCOA, 1993). The United States Environmental Protection Agency (U.S. EPA) estimated an oral Reference Dose (RfD) as 5 x 10⁻³ milligrams per kilogram per day (mg/kg/d), based on reproductive effects. The U.S. EPA estimates that consumption of this dose or less, over a lifetime, would not likely result in the occurrence of chronic, non-cancer effects (U.S. EPA, 1995a).

Cancer: The U.S. EPA and IARC have not determined a cancer classification for o-chlorophenol (U.S. EPA, 1995a; IARC, 1987a).

2,3,4,6-Tetrachlorophenol

Non-Cancer: Exposure to 2,3,4,6-tetrachlorophenol dust can cause eye irritation (HSDB, 1995). A chronic non-cancer Reference Exposure Level (REL) of 88 μ g/m³ is listed for 2,3,4,6-tetrachlorophenol in the California Air Pollution Control Officers Association Air Toxics "Hot Spots" Program, Revised 1992 Risk Assessment Guidelines. The toxicological endpoints considered were the gastrointestinal system and liver (CAPCOA 1993). The U.S. EPA (1995) established an oral Reference Dose (RfD) of 3 x 10^{-2} mg/kg/d, based on liver effects. The U.S. EPA estimates that consumption of this dose or less, over a lifetime, would not likely result in the occurrence of chronic, non-cancer effects (U.S. EPA, 1995a).

Cancer: The carcinogenicity of 2,3,4,6-tetrachlorophenol has not been evaluated by the U.S. EPA (U.S. EPA, 1995a). The IARC has classified 2,3,4,6-tetrachlorophenol in Group 2B: Possible human carcinogen, based on its identity as a chlorophenol, for which human data are limited (IARC, 1987a).